

09/06/2006

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Welcome to STN International! Enter x:x

LOGINID:SSPTASXY1626

PASSWORD:

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* * * * * Welcome to STN International * * * * *

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	JAN 17	Pre-1988 INPI data added to MARPAT
NEWS	4	FEB 21	STN AnaVist, Version 1.1, lets you share your STN AnaVist visualization results
NEWS	5	FEB 22	The IPC thesaurus added to additional patent databases on STN
NEWS	6	FEB 22	Updates in EPFULL; IPC 8 enhancements added
NEWS	7	FEB 27	New STN AnaVist pricing effective March 1, 2006
NEWS	8	MAR 03	Updates in PATDPA; addition of IPC 8 data without attributes
NEWS	9	MAR 22	EMBASE is now updated on a daily basis
NEWS	10	APR 03	New IPC 8 fields and IPC thesaurus added to PATDPAFULL
NEWS	11	APR 03	Bibliographic data updates resume; new IPC 8 fields and IPC thesaurus added in PCTFULL
NEWS	12	APR 04	STN AnaVist \$500 visualization usage credit offered
NEWS	13	APR 12	LINSPEC, learning database for INSPEC, reloaded and enhanced
NEWS	14	APR 12	Improved structure highlighting in FQHIT and QHIT display in MARPAT
NEWS	15	APR 12	Derwent World Patents Index to be reloaded and enhanced during second quarter; strategies may be affected
NEWS	16	MAY 10	CA/CAPLUS enhanced with 1900-1906 U.S. patent records
NEWS	17	MAY 11	KOREAPAT updates resume
NEWS	18	MAY 19	Derwent World Patents Index to be reloaded and enhanced
NEWS	19	MAY 30	IPC 8 Rolled-up Core codes added to CA/CAPLUS and USPATFULL/USPAT2
NEWS	20	MAY 30	The F-Term thesaurus is now available in CA/CAPLUS
NEWS EXPRESS			FEBRUARY 15 CURRENT VERSION FOR WINDOWS IS V8.01a, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 19 DECEMBER 2005. V8.0 AND V8.01 USERS CAN OBTAIN THE UPGRADE TO V8.01a AT http://download.cas.org/express/v8.0-Discover/
NEWS HOURS			STN Operating Hours Plus Help Desk Availability
NEWS LOGIN			Welcome Banner and News Items
NEWS IPC8			For general information regarding STN implementation of IPC 8
NEWS X25			X.25 communication option no longer available after June 2006

Enter NEWS followed by the item number or name to see news on that specific topic.

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09/06/2006

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 14:21:48 ON 01 JUN 2006

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 14:21:53 ON 01 JUN 2006

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Property values tagged with IC are from the ZIC/VINITI data file
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STRUCTURE FILE UPDATES: 31 MAY 2006 HIGHEST RN 886358-42-5

DICTIONARY FILE UPDATES: 31 MAY 2006 HIGHEST RN 886358-42-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*

Structure search iteration limits have been increased. See HELP SLIMITS
for details.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

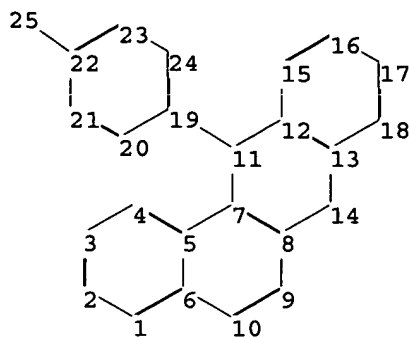
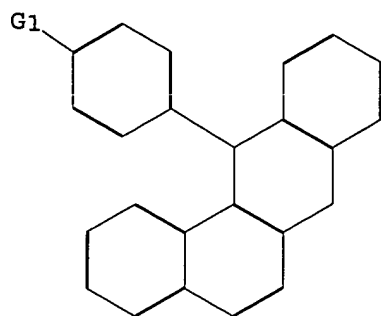
<http://www.cas.org/ONLINE/UG/regprops.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10527527c.str

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09/06/2006



chain nodes :

25

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24

chain bonds :

11-19 22-25

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 7-11 8-9 8-14 9-10 11-12 12-13 12-15 13-14 13-18 15-16 16-17 17-18 19-20 19-24 20-21 21-22 22-23 23-24

exact/norm bonds :

7-11 8-14 11-12 13-14 22-25

exact bonds :

11-19

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 12-13 12-15 13-18 15-16 16-17 17-18 19-20 19-24 20-21 21-22 22-23 23-24

G1:O,S,N,CH2

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:CLASS

L1 STRUCTURE UPLOADED

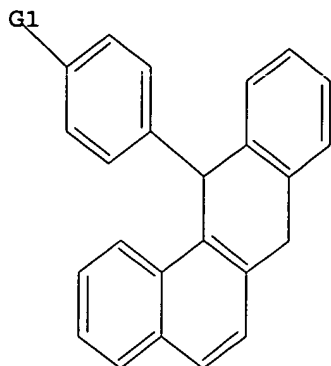
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L1 HAS NO ANSWERS

L1 STR

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G1 O,S,N,CH2

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 14:22:20 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 1636 TO ITERATE

100.0% PROCESSED 1636 ITERATIONS

2 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 30294 TO 35146

PROJECTED ANSWERS: 2 TO 124

L2 2 SEA SSS SAM L1

=> s l1 full

FULL SEARCH INITIATED 14:22:26 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 32812 TO ITERATE

100.0% PROCESSED 32812 ITERATIONS

33 ANSWERS

SEARCH TIME: 00.00.01

L3 33 SEA SSS FUL L1

=> file hcaplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

166.94

167.15

FILE 'HCAPLUS' ENTERED AT 14:22:32 ON 01 JUN 2006

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FILE COVERS 1907 - 1 Jun 2006 VOL 144 ISS 23

FILE LAST UPDATED: 31 May 2006 (20060531/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3

L4 16 L3

=> d ed abs ibib hitstr 1-16

L4 ANSWER 1 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 21 Sep 2004

AB For selective estrogen receptor modulators (SERMs), the orientation of the basic side chain relative to the SERM core has a significant impact on function. The synthesis and biol. evaluation of two series of SERMs are disclosed, where the ligand side chain is constrained to adopt a defined orientation. Compds. where the side chain is forced into the plane of the SERM core have a different profile compared to those compds. where the side chain is pseudo-orthogonal, particularly with regard to antagonism of estradiol action on an Ishikawa uterine cell line.

ACCESSION NUMBER: 2004:767285 HCAPLUS

DOCUMENT NUMBER: 141:410789

TITLE: Benzothiophene and naphthalene derived constrained SERMs

AUTHOR(S): Wallace, Owen B.; Bryant, Henry U.; Shetler, Pamela K.; Adrian, Mary D.; Geiser, Andrew G.

CORPORATE SOURCE: Lilly Research Laboratories, Eli Lilly and Company, Lilly Corporate Center, Indianapolis, IN, 46285, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (2004), 14(20), 5103-5106

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:410789

IT 676456-49-8P 676456-50-1P

RL: PAC (Pharmacological activity); PUR (Purification or recovery); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (preparation of piperazinoethoxyphenylbenzonaphthothiophenes and -benzanthracenes as selective estrogen receptor modulators)

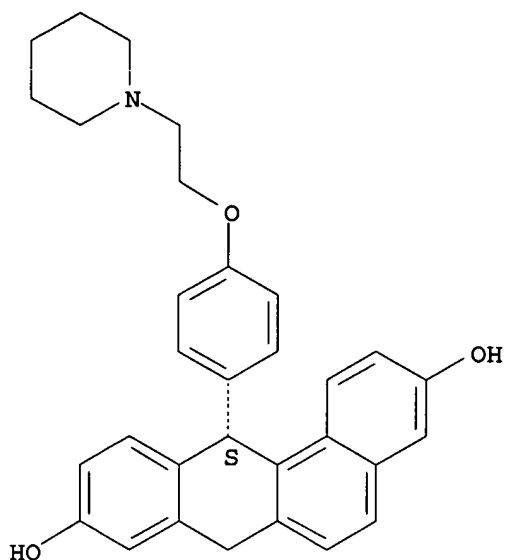
RN 676456-49-8 HCAPLUS

CN Benz[a]anthracene-3,9-diol, 7,12-dihydro-12-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, (12S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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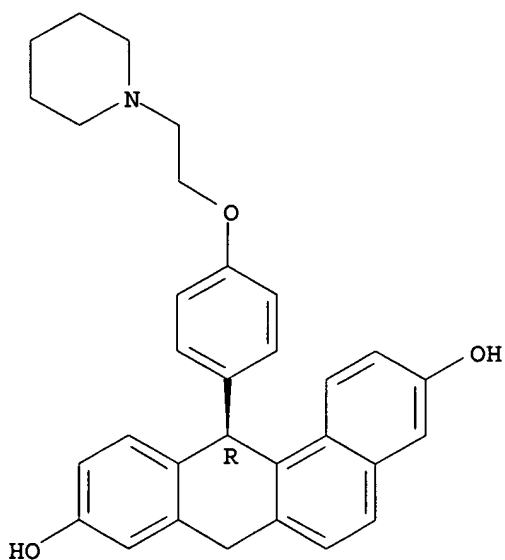
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RN 676456-50-1 HCAPLUS

CN Benz[a]anthracene-3,9-diol, 7,12-dihydro-12-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, (12R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 676456-43-2P 676456-46-5P 676456-51-2P

676456-53-4P 791837-75-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

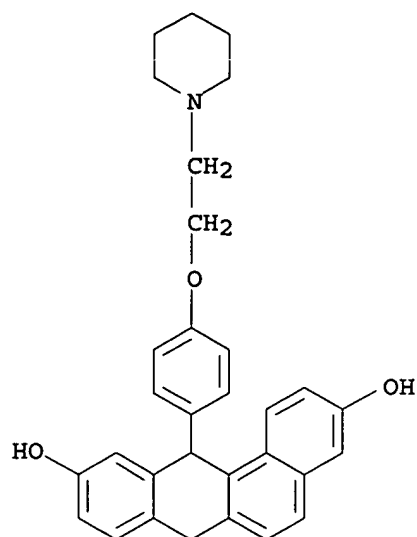
(preparation of piperazinoethoxyphenylbenzonaphthothiophenes and -benzanthracenes as selective estrogen receptor modulators)

RN 676456-43-2 HCAPLUS

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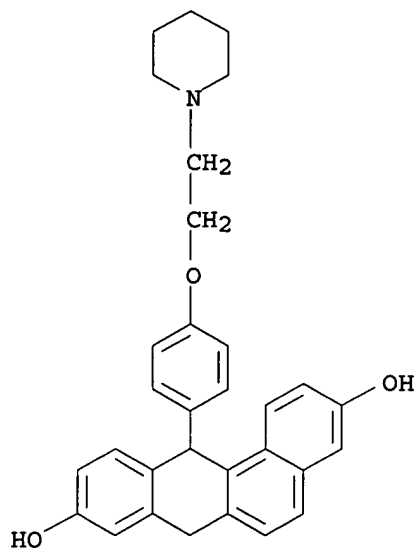
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RN 676456-46-5 HCAPLUS

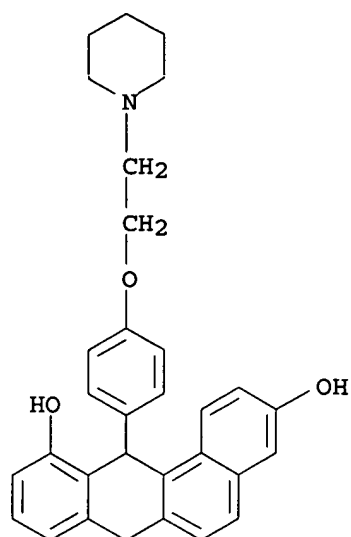
CN Benz[a]anthracene-3,9-diol, 7,12-dihydro-12-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)



RN 676456-51-2 HCAPLUS

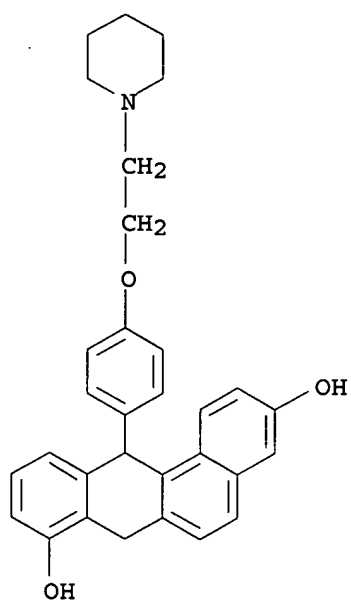
CN Benz[a]anthracene-3,11-diol, 7,12-dihydro-12-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)

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RN 676456-53-4 HCAPLUS

CN Benz[a]anthracene-3,8-diol, 7,12-dihydro-12-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)

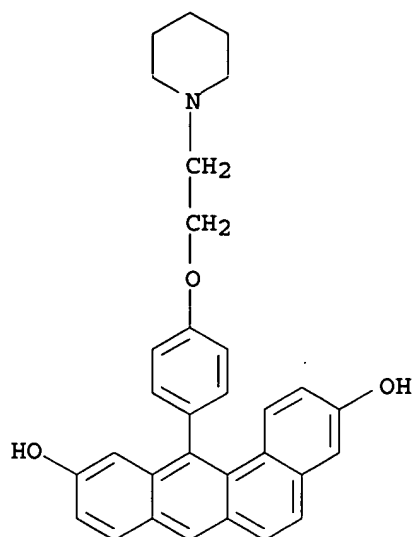


RN 791837-75-7 HCAPLUS

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(CA INDEX NAME)

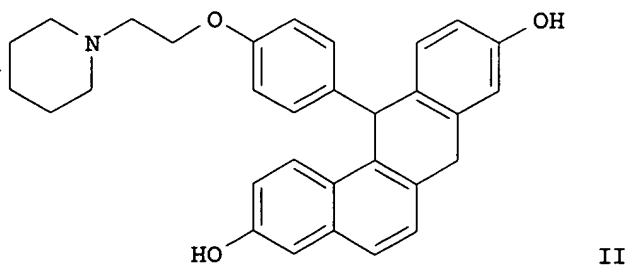
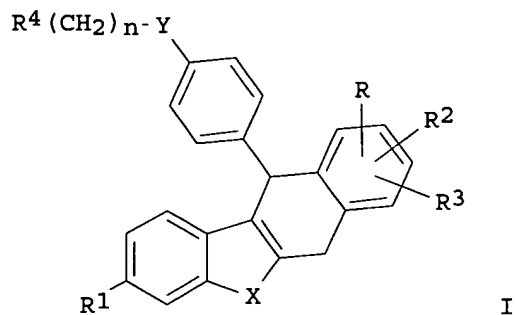
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REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 09 Apr 2004
GI



AB Dihydro-dibenzo(a)anthracenes of formula I [R1 = H, OH, alkoxy, benzoyloxy, acyloxy, OSO2alkyl, etc.; R, R2, R3 = H, OH, alkoxy, benzoyloxy, acyloxy, OSO2alkyl, halo; R4 = 1-piperidinyl, 1-pyrrolidinyl, methyl-1-pyrrolidinyl, dimethyl-1-pyrrolidinyl, 4-morpholino, dimethylamino, diethylamino, diisopropylamino, or 1-hexamethyleneimino; n

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09/06/2006

= 2-3; X = S, CH=CH; Y = O, S, NH, NMe, CH₂] are prepared for pharmaceutical compns., optionally in combination with estrogen and progestin, for inhibiting a disease associated with estrogen deprivation or a disease associated with an aberrant physiolo. response to endogenous estrogen. Thus, II.TFA was prepared from (2,6-dimethoxynaphthalen-1-yl)-[4-(2-piperidin-1-ylethoxy)phenyl]methanone and 3-methoxybenzylzinc chloride. II had IC₅₀ of 2 nM against MCF-7 breast adenocarcinoma cells.

ACCESSION NUMBER: 2004:292023 HCAPLUS
DOCUMENT NUMBER: 140:303419
TITLE: Preparation of dihydro-dibenzo(a)anthracenes as selective estrogen receptor modulators
INVENTOR(S): Wallace, Owen Brendan
PATENT ASSIGNEE(S): Eli Lilly and Company, USA
SOURCE: PCT Int. Appl., 58 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004029047	A1	20040408	WO 2003-US26304	20030922
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
CA 2497627	AA	20040408	CA 2003-2497627	20030922
AU 2003265581	A1	20040419	AU 2003-265581	20030922
EP 1546139	A1	20050629	EP 2003-798700	20030922
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK			
BR 2003014594	A	20050809	BR 2003-14594	20030922
JP 2006508066	T2	20060309	JP 2004-539841	20030922
PRIORITY APPLN. INFO.:			US 2002-413609P	P 20020925
			WO 2003-US26304	W 20030922

OTHER SOURCE(S): MARPAT 140:303419

IT 676456-38-5P 676456-39-6P 676456-41-0P
676456-43-2P 676456-44-3P 676456-46-5P
676456-47-6P 676456-49-8P 676456-50-1P
676456-51-2P 676456-52-3P 676456-53-4P

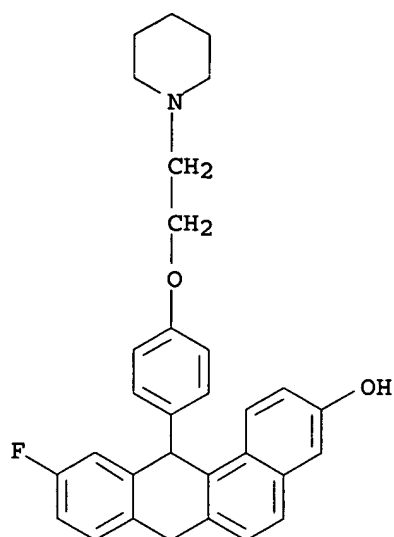
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of dihydro-dibenzoanthracenes as selective estrogen receptor modulators)

RN 676456-38-5 HCAPLUS

CN Benz[a]anthracen-3-ol, 10-fluoro-7,12-dihydro-12-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)

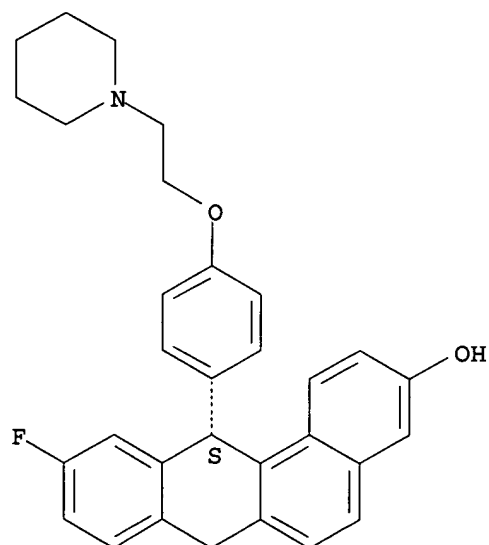
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RN 676456-39-6 HCAPLUS

CN Benz[a]anthracen-3-ol, 10-fluoro-7,12-dihydro-12-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, (12S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



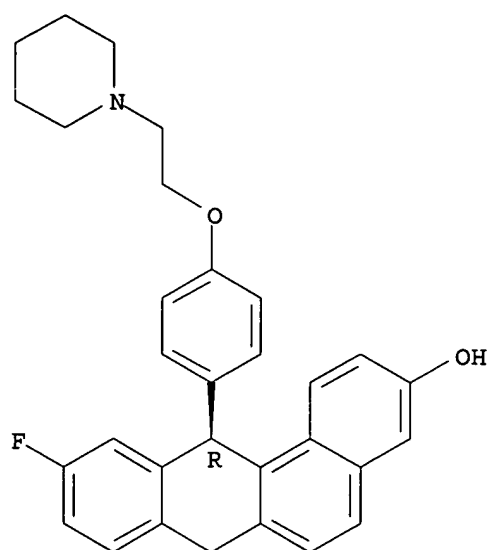
RN 676456-41-0 HCAPLUS

CN Benz[a]anthracen-3-ol, 10-fluoro-7,12-dihydro-12-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, (12R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

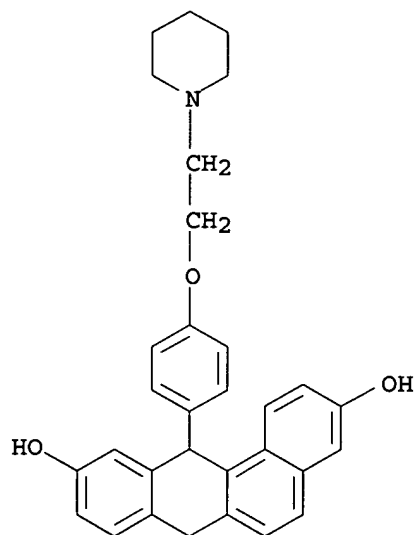
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RN 676456-43-2 HCAPLUS

CN Benz[a]anthracene-3,10-diol, 7,12-dihydro-12-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)



RN 676456-44-3 HCAPLUS

CN Benz[a]anthracene-3,10-diol, 7,12-dihydro-12-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, trifluoroacetate (salt) (9CI) (CA INDEX NAME)

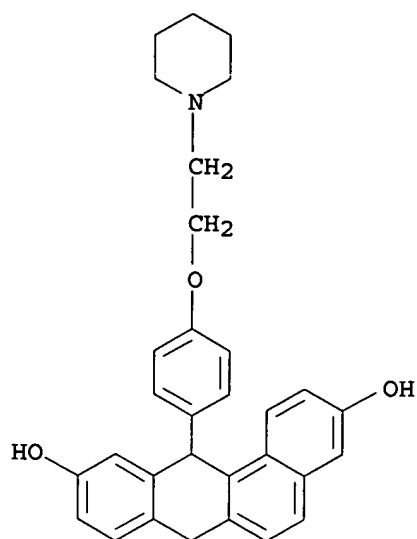
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CRN 676456-43-2

CMF C31 H31 N O3

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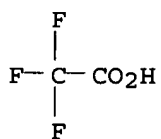
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CM 2

CRN 76-05-1

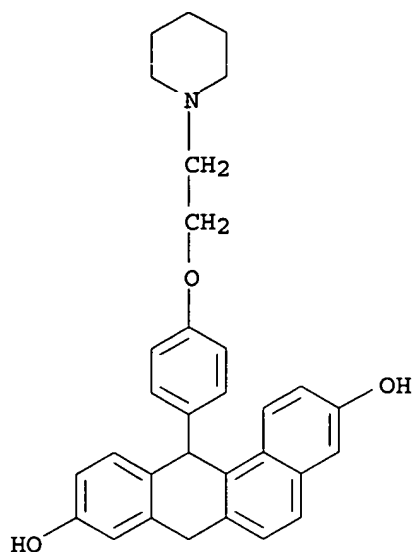
CMF C2 H F3 O2



RN 676456-46-5 HCAPLUS

CN Benz[a]anthracene-3,9-diol, 7,12-dihydro-12-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)

09/06/2006



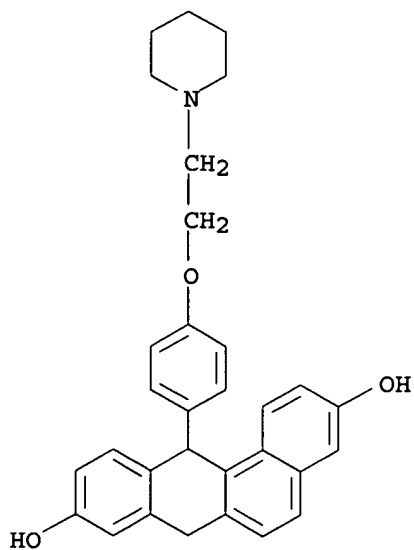
RN 676456-47-6 HCAPLUS

CN Benz[a]anthracene-3,9-diol, 7,12-dihydro-12-[4-[2-(1-piperidinyloxy)phenyl]-, trifluoroacetate (salt) (9CI) (CA INDEX NAME)

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CRN 676456-46-5

CMF C31 H31 N O3



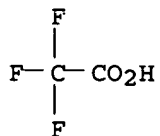
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CRN 76-05-1

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09/06/2006

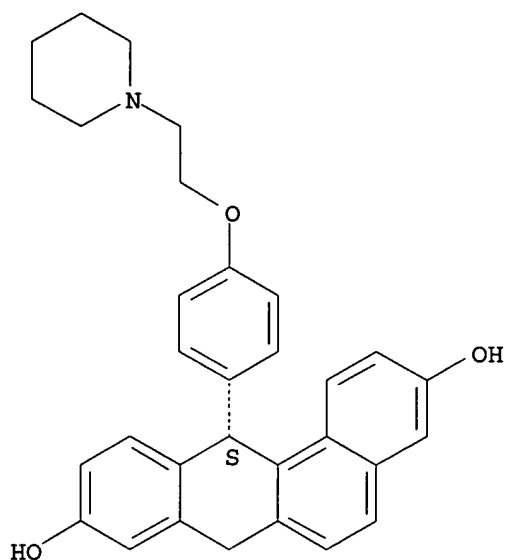
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RN 676456-49-8 HCAPLUS

CN Benz[a]anthracene-3,9-diol, 7,12-dihydro-12-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, (12S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

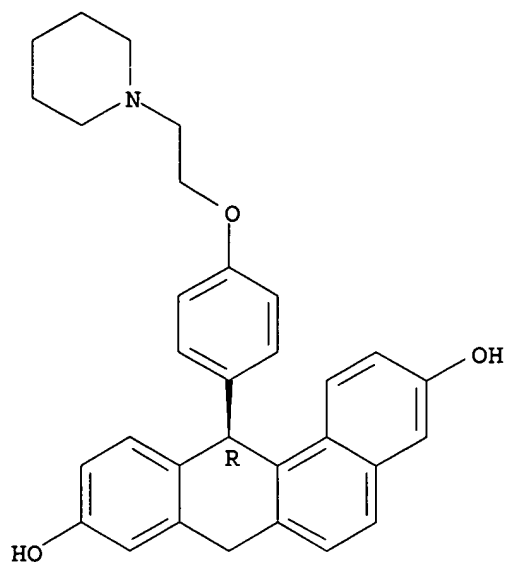


RN 676456-50-1 HCAPLUS

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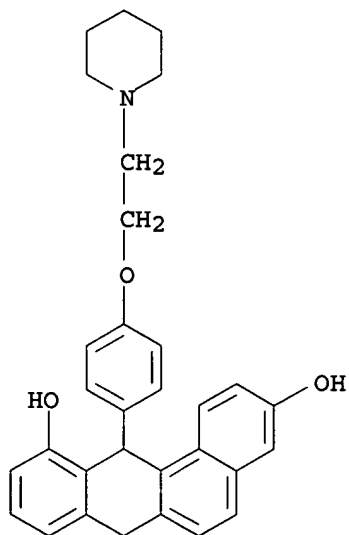
Absolute stereochemistry.

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RN 676456-51-2 HCAPLUS

CN Benz[a]anthracene-3,11-diol, 7,12-dihydro-12-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)



RN 676456-52-3 HCAPLUS

CN Benz[a]anthracene-3,11-diol, 7,12-dihydro-12-[4-[2-(1-piperidinyl)ethoxy]phenyl]-, trifluoroacetate (salt) (9CI) (CA INDEX NAME)

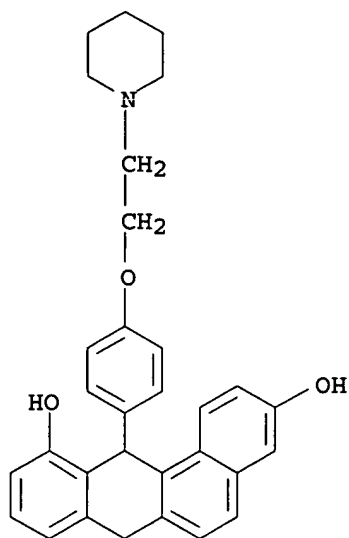
CM 1

CRN 676456-51-2

CMF C31 H31 N O3

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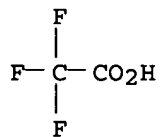
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CM 2

CRN 76-05-1

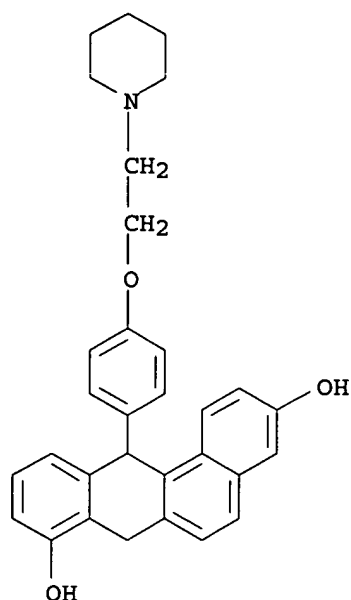
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RN 676456-53-4 HCAPLUS

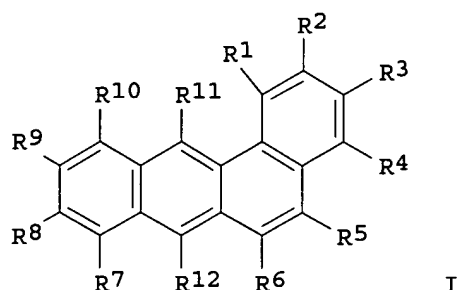
CN Benz[a]anthracene-3,8-diol, 7,12-dihydro-12-[4-[2-(1-piperidinyl)ethoxy]phenyl]- (9CI) (CA INDEX NAME)

09/06/2006



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 27 Jun 2000
GI



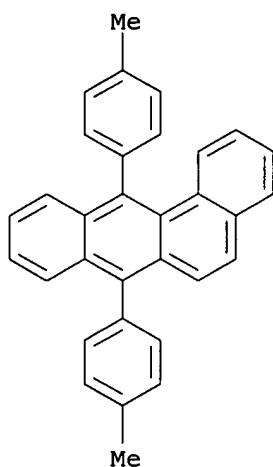
AB The invention refers to a luminescent material comprising a benzanthracene I [R1-11 = H, alkyl, alkoxy, R11,12 = Ph, naphthyl, anthryl, phenanthryl, biphenyl, or terphenyl which may be contain alkyl of alkoxy substituents.].

ACCESSION NUMBER: 2000:428078 HCAPLUS
DOCUMENT NUMBER: 133:65844
TITLE: Luminescent material
INVENTOR(S): Sakaki, Yuichi; Nagasaki, Yoshinori
PATENT ASSIGNEE(S): Toppan Printing Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

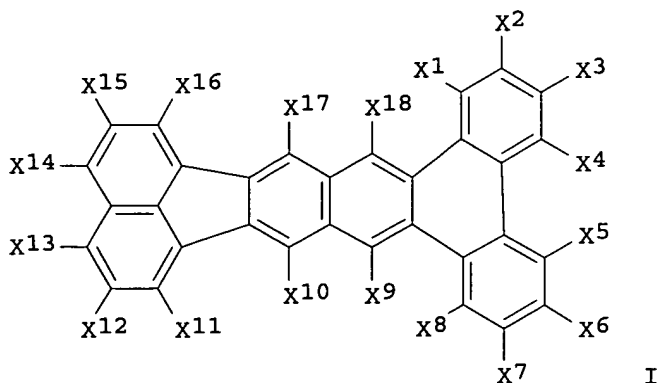
Young, Shawquia

09/06/2006

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2000178548	A2	20000627	JP 1998-358184	19981216
PRIORITY APPLN. INFO.:			JP 1998-358184	19981216
OTHER SOURCE(S):	MARPAT 133:65844			
IT 277754-42-4				
RL: DEV (Device component use); USES (Uses)				
	(luminescent material)			
RN 277754-42-4 HCAPLUS				
CN Benz[a]anthracene, 7,12-bis(4-methylphenyl) - (9CI)			(CA INDEX NAME)	



L4 ANSWER 4 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 03 Feb 1999
GI



AB The device has a layer containing ≥ 1 fluorantheno[8,9-b]triphenylene derivative (I; X1-10 = H, halo, straight, branched or cyclic alkyl or alkoxy, or (un)substituted aryl) between a pair of electrodes. The device shows

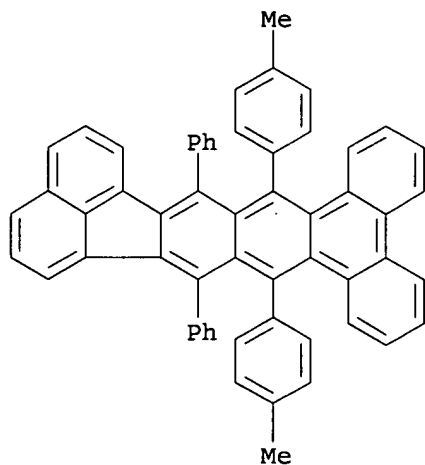
Young, Shawquia

09/06/2006

high emission.

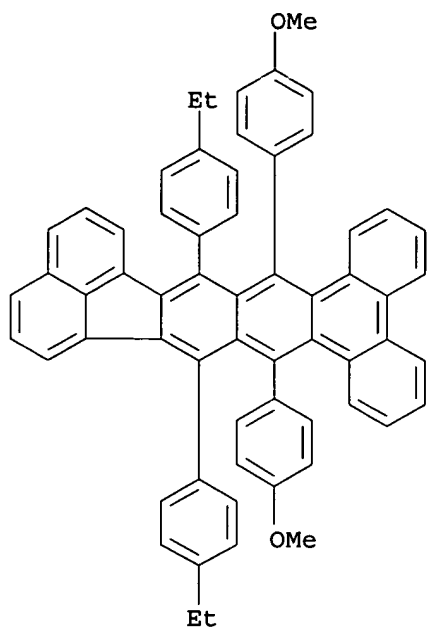
ACCESSION NUMBER: 1999:72210 HCAPLUS
DOCUMENT NUMBER: 130:175060
TITLE: Organic electroluminescent device containing
fluorantheno[8,9-b]triphenylene derivative
INVENTOR(S): Nakatsuka, Masakatsu; Kitamoto, Noriko
PATENT ASSIGNEE(S): Mitsui Chemicals Inc., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11026158	A2	19990129	JP 1997-175909	19970701
JP 3727143	B2	20051214		
PRIORITY APPLN. INFO.:			JP 1997-175909	19970701
OTHER SOURCE(S):		MARPAT 130:175060		
IT 220345-16-4 220345-17-5 220345-20-0				
RL: DEV (Device component use); USES (Uses)				
(organic electroluminescent device containing				
fluorantheno[8,9-b]triphenylene				
derivative)				
RN 220345-16-4 HCAPLUS				
CN Fluorantheno[8,9-b]triphenylene, 8,17-bis(4-methylphenyl)-7,18-diphenyl-				
(9CI) (CA INDEX NAME)				

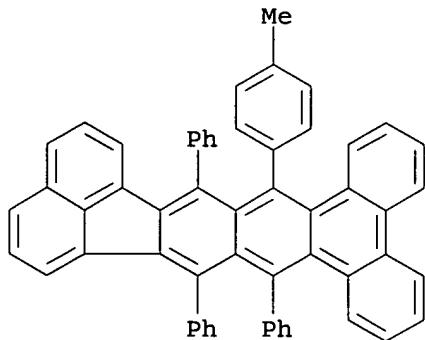


RN 220345-17-5 HCAPLUS
CN Fluorantheno[8,9-b]triphenylene, 7,18-bis(4-ethylphenyl)-8,17-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

09/06/2006



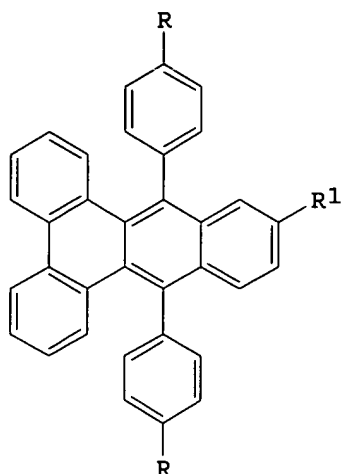
RN 220345-20-0 HCAPLUS
CN Fluorantheno[8,9-b]triphenylene, 8-(4-methylphenyl)-7,17,18-triphenyl-
(9CI) (CA INDEX NAME)



L4 ANSWER 5 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 09 Feb 1991
GI

Young, Shawquia

09/06/2006



AB The preparation of ten 9,14-diphenylbenzo[b]triphenylene derivs. I (R = H, NO₂, OMe, SMe, Cl, Br, CF₃, cyano, Me; R₁ = H, Me) was described. The crystal and mol. structure and end-to-end twists in I (same R, R₁) were determined and the effects of substituents and crystal packing forces on the solid-state conformations were discussed. The presence of electronic substituent effects and their bearing on the magnitude of hydrogen-to-arene nonbonded repulsions was discussed.

ACCESSION NUMBER: 1991:42249 HCAPLUS

DOCUMENT NUMBER: 114:42249

TITLE: A study of substituent effects on hydrogen-to-arene nonbonded interactions

AUTHOR(S): L'Esperance, Robert P.; Van Engen, Donna; Dayal, Rajeev; Pascal, Robert A., Jr.

CORPORATE SOURCE: Dep. Chem., Princeton Univ., Princeton, NJ, 08544, USA

SOURCE: Journal of Organic Chemistry (1991), 56(2), 688-94

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 114:42249

IT 87771-74-2P 87771-75-3P 131273-85-3P

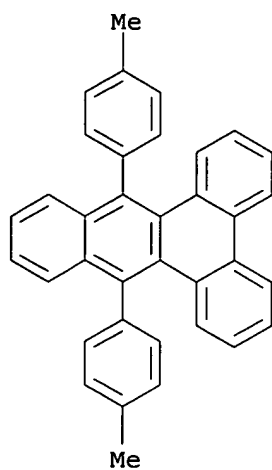
131273-86-4P 131273-91-1P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure of, effect of substituents and crystal packing forces on solid-state conformation of)

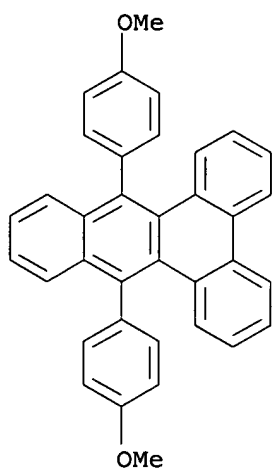
RN 87771-74-2 HCAPLUS

CN Benzo[b]triphenylene, 9,14-bis(4-methylphenyl)- (9CI) (CA INDEX NAME)

09/06/2006



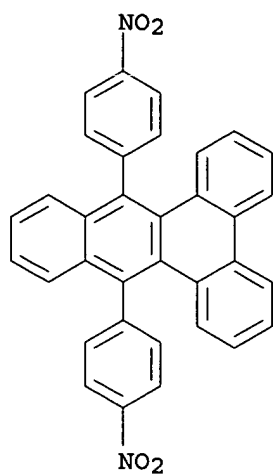
RN 87771-75-3 HCAPLUS
CN Benzo[b]triphenylene, 9,14-bis(4-methoxyphenyl) - (9CI) (CA INDEX NAME)



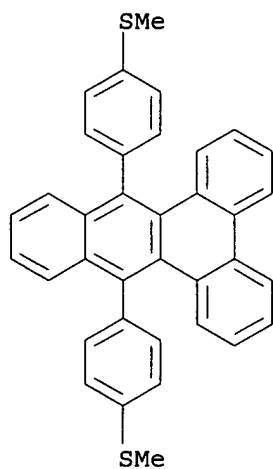
RN 131273-85-3 HCAPLUS
CN Benzo[b]triphenylene, 9,14-bis(4-nitrophenyl) - (9CI) (CA INDEX NAME)

Young, Shawquia

09/06/2006



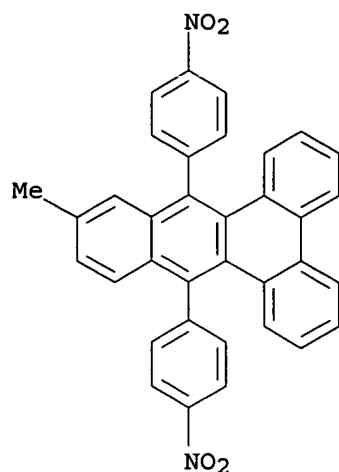
RN 131273-86-4 HCAPLUS
CN Benzo[b]triphenylene, 9,14-bis[4-(methylthio)phenyl] - (9CI) (CA INDEX NAME)



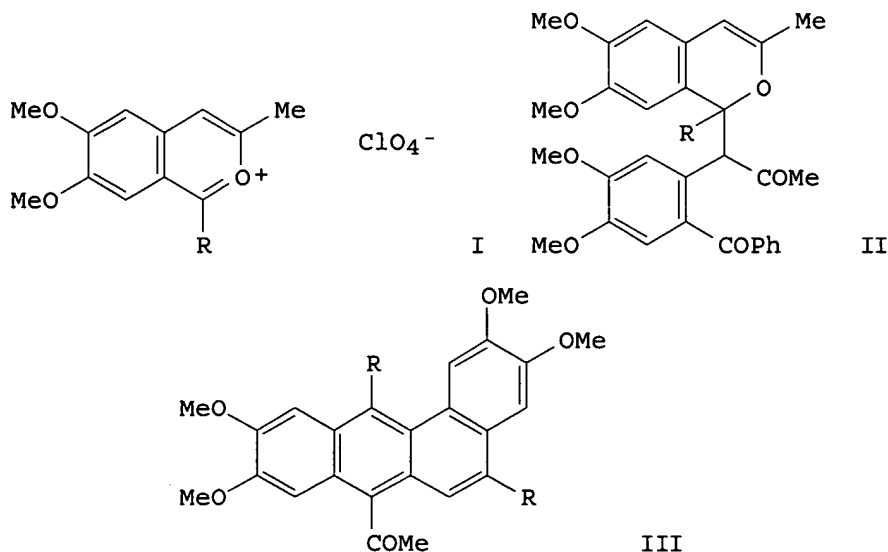
RN 131273-91-1 HCAPLUS
CN Benzo[b]triphenylene, 11-methyl-9,14-bis(4-nitrophenyl) - (9CI) (CA INDEX NAME)

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09/06/2006



L4 ANSWER 6 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 21 Jul 1989
GI



AB Treatment of benzopyrylium salts I (R = Ph, p-anisyl) with NaOH or KOH in H₂O-Et₂O afforded dimers II, which cyclized to benz[a]anthracenes III on treatment with Me₂CHOH-NaOH in H₂O and then acidolysis with glacial AcOH. The acetyl group in III (R = Ph) was cleaved by CF₃CO₂H.

ACCESSION NUMBER: 1989:423196 HCAPLUS

DOCUMENT NUMBER: 111:23196

TITLE: 2-Benzopyrylium salts. 33. 4,1'-Dimerization of

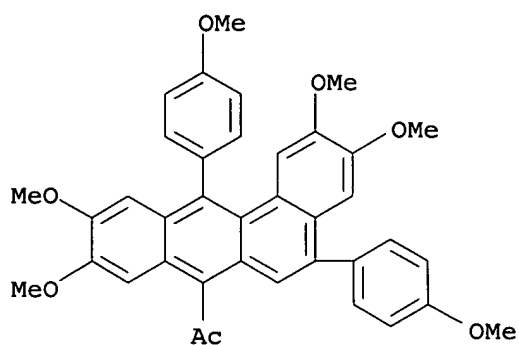
2-benzopyrylium salts; formation of benz[a]anthracenes

AUTHOR(S): Zhdanov, Yu. A.; Verin, S. V.; Korobka, I. V.;

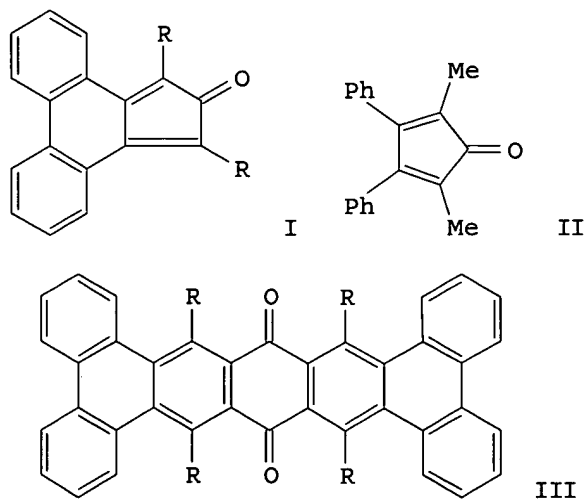
Young, Shawquia

09/06/2006

CORPORATE SOURCE: Kuznetsov, E. V.
SOURCE: Rostov. Gos. Univ., Rostov, 344071, USSR
Khimiya Geterotsiklicheskikh Soedinenii (1988), (9),
1185-9
CODEN: KGSSAQ; ISSN: 0453-8234
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 111:23196
IT 121262-27-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 121262-27-9 HCAPLUS
CN Ethanone, 1-[2,3,9,10-tetramethoxy-5,12-bis(4-
methoxyphenyl)benz[a]anthracen-7-yl]- (9CI) (CA INDEX NAME)



L4 ANSWER 7 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 18 May 1985
GI

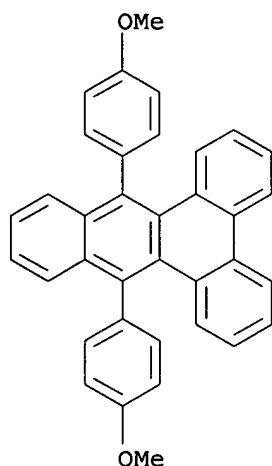


AB Polycyclic aromatic quinones were prepared by Diels-Alder reaction of
Young, Shawquia

09/06/2006

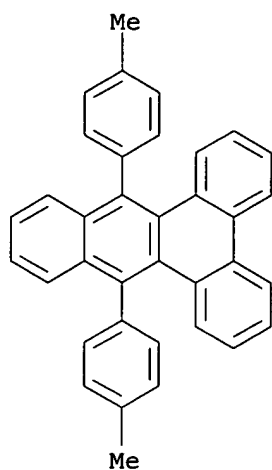
cyclopentadienones I (R = Ph, 4-MeC₆H₄, 4-MeOC₆H₄, 3,4-Me₂C₆H₃) and II with benzoquinone and naphthaquinone. The monoadducts, when used as dienophiles, condense with I, affording a new series of quinones III.

ACCESSION NUMBER: 1985:166436 HCAPLUS
DOCUMENT NUMBER: 102:166436
TITLE: Polycyclic aromatic compounds: a new synthesis of highly arylated quinones by Diels-Alder reaction
AUTHOR(S): Mondal, S.; Bhattacharya, A. J.
CORPORATE SOURCE: Dep. Chem., Univ. Burdwan, Burdwan, 713 104, India
SOURCE: Current Science (1984), 53(23), 1229-32
CODEN: CUSCAM; ISSN: 0011-3891
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 102:166436
IT 87771-75-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and Diels-Alder reaction of, with cyclopentadienone derivs.)
RN 87771-75-3 HCAPLUS
CN Benzo[b]triphenylene, 9,14-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

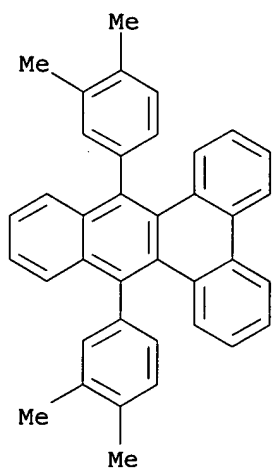


IT 87771-74-2P 87771-76-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 87771-74-2 HCAPLUS
CN Benzo[b]triphenylene, 9,14-bis(4-methylphenyl)- (9CI) (CA INDEX NAME)

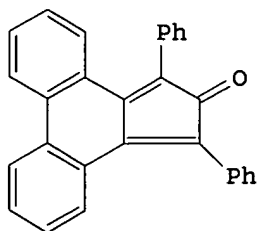
09/06/2006



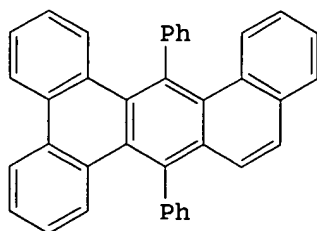
RN 87771-76-4 HCAPLUS
CN Benzo[b]triphenylene, 9,14-bis(3,4-dimethylphenyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 8 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN
GI



I



II

Young, Shawquia

09/06/2006

AB Diels-Alder cycloaddn. of cyclopentadienones, e.g., I with dienophiles, e.g., 1-chloro-3,4-dihydronaphthalene and 5,6-dimethyl-1-chloro-3(H)-indene, gave polycyclic aromatic compds., e.g., II.

ACCESSION NUMBER: 1984:610704 HCAPLUS

DOCUMENT NUMBER: 101:210704

TITLE: Polycyclic aromatic compounds: synthesis of polycyclics containing anthracene, phenanthrene and fluorene nucleus

AUTHOR(S): Mondal, S.; Bhattacharya, A. J.

CORPORATE SOURCE: Dep. Chem., Univ. Burdwan, Burdwan, 713 104, India

SOURCE: Current Science (1984), 53(13), 676-9

CODEN: CUSCAM; ISSN: 0011-3891

DOCUMENT TYPE: Journal

LANGUAGE: English

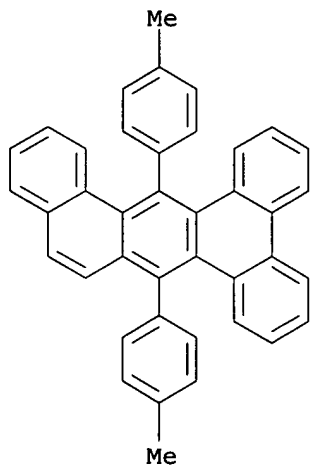
OTHER SOURCE(S): CASREACT 101:210704

IT 93193-98-7P 93193-99-8P 93194-00-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by Diels-Alder cycloaddn. reaction)

RN 93193-98-7 HCAPLUS

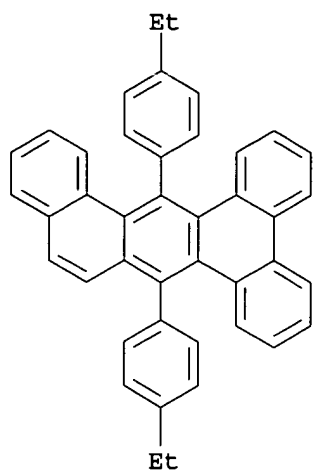
CN Naphtho[1,2-b]triphenylene, 9,16-bis(4-methylphenyl)- (9CI) (CA INDEX NAME)



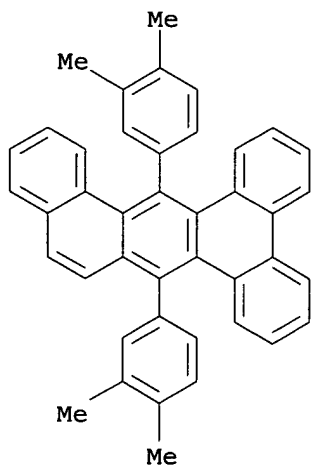
RN 93193-99-8 HCAPLUS

CN Naphtho[1,2-b]triphenylene, 9,16-bis(4-ethylphenyl)- (9CI) (CA INDEX NAME)

09/06/2006



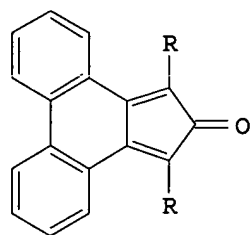
RN 93194-00-4 HCAPLUS
CN Naphtho[1,2-b]triphenylene, 9,16-bis(3,4-dimethylphenyl)- (9CI) (CA INDEX NAME)



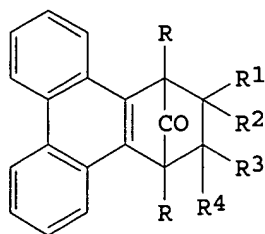
L4 ANSWER 9 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 12 May 1984
GI

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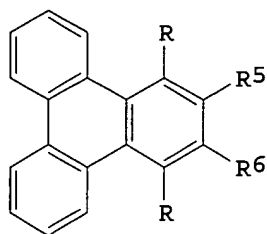
09/06/2006



I



II



III

AB Diels-Alder cycloaddn. of cyclopentaphenanthranones I (R = Ph, C₆H₄Me-4, C₆H₄OMe-4, C₆H₃Me₂-3,4) with dienophiles norbornadiene, indene, PhC.tplbond.CPh, and benzyne gave methanodibenzoanthracenes II (R₁ = R₃ = H, R₂R₄ = 3,5-cyclopentenyl, 2-C₆H₄CH₂; R₂ = R₄ = Ph; R₁R₃ = bond, R₂R₄ = CH:CHCH:CH) resp. Thermal treatment of II (R₂R₄ = 2-C₆H₄CH₂) gave of CO and/or cyclopentadiene to give triphenylenes III (R₅ = R₆ = H, Ph; R₅R₆ = CH:CHCH:CH). Treating I with 1-chloro-6-methyl-3(H)indene gave III (R₅R₆ = C₆H₃MeCH₂-3,6) directly.

ACCESSION NUMBER: 1983:594595 HCAPLUS

DOCUMENT NUMBER: 99:194595

TITLE: Polycyclic aromatic compounds: Part VIII. A new synthesis of polycyclics containing phenanthrene nucleus

AUTHOR(S): Mondal, S.; Bandyopadhyay, T. K.; Bhattacharya, A. J.

CORPORATE SOURCE: Dep. Chem., Burdwan Univ., Burdwan, 713 104, India

SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1983), 22B(5), 448-52

CODEN: IJSBDB; ISSN: 0376-4699

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 99:194595

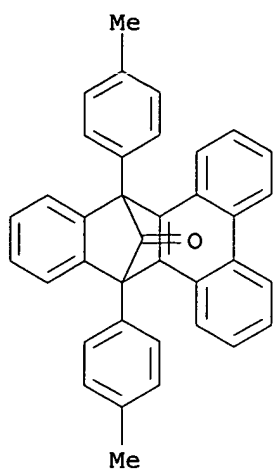
IT 87771-71-9P 87771-72-0P 87771-73-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and decarbonylation of)

RN 87771-71-9 HCAPLUS

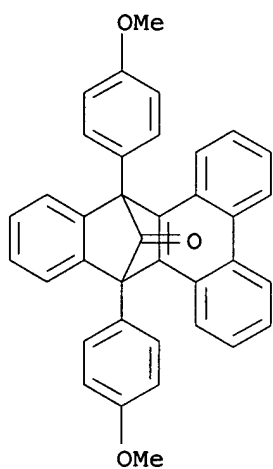
CN 9,14-Methanobenzo[b]triphenylen-15-one, 9,14-dihydro-9,14-bis(4-methylphenyl)- (9CI) (CA INDEX NAME)

09/06/2006



RN 87771-72-0 HCAPLUS

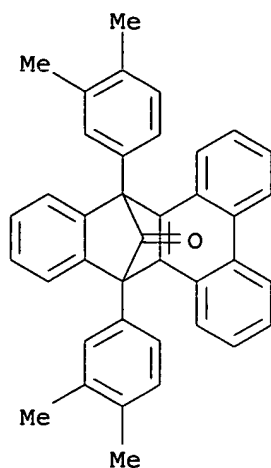
CN 9,14-Methanobenzo[b]triphenylen-15-one, 9,14-dihydro-9,14-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



RN 87771-73-1 HCAPLUS

CN 9,14-Methanobenzo[b]triphenylen-15-one, 9,14-bis(3,4-dimethylphenyl)-9,14-dihydro- (9CI) (CA INDEX NAME)

09/06/2006

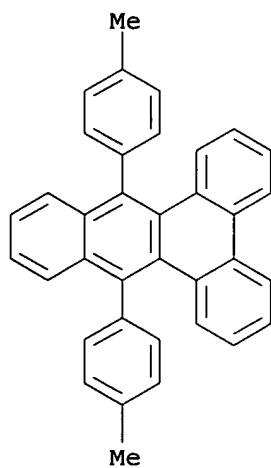


IT 87771-74-2P 87771-75-3P 87771-76-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 87771-74-2 HCAPLUS

CN Benzo[b]triphenylene, 9,14-bis(4-methylphenyl)- (9CI) (CA INDEX NAME)

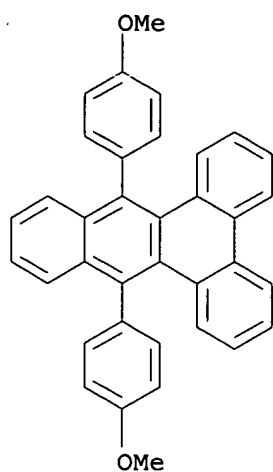


RN 87771-75-3 HCAPLUS

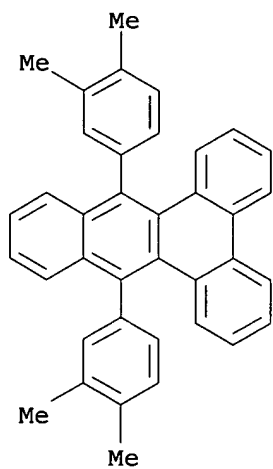
CN Benzo[b]triphenylene, 9,14-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

Young, Shawquia

09/06/2006



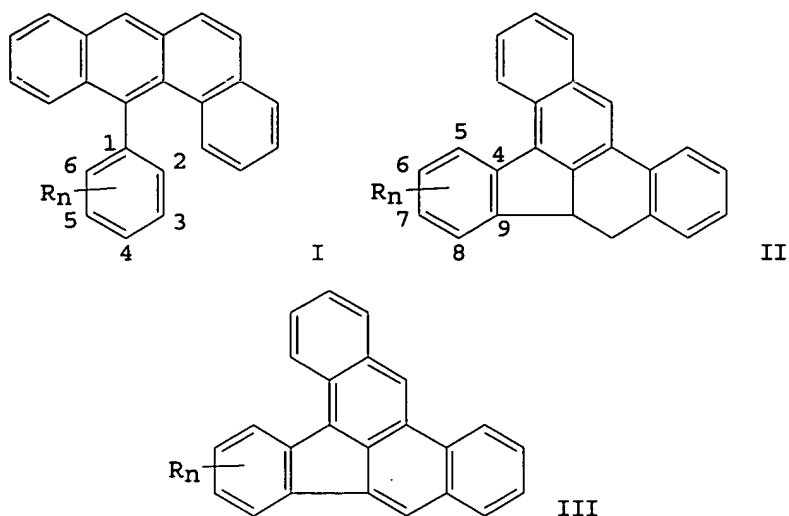
RN 87771-76-4 HCAPLUS
CN Benzo[b]triphenylene, 9,14-bis(3,4-dimethylphenyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 10 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 12 May 1984
GI

Young, Shawquia

09/06/2006



AB Treatment of phenylbenzanthracenes I (R_n = 2-, 3-, 4-Me, 3,4-, 3,5-, 2,3-, 2,4-Me₂) with AlCl₃ gave 30-88% II (R_n = 5-, 7-, 8-Me, 7,8-, 6,8-, 5,6-, 5,7-Me₂), which were aromatized with 2,3-dichloro-5,6-dicyanobenzoquinone to give III quant.

ACCESSION NUMBER: 1979:203754 HCAPLUS

DOCUMENT NUMBER: 90:203754

TITLE: Modified Scholl synthesis of substituted dibenzo[a,e]fluoranthenes and their dihydro intermediates

AUTHOR(S): Youssef, Abdullatif K.; Vingiello, Frank A.; Ogliaruso, Michael A.

CORPORATE SOURCE: Fac. Sci., Tishreen Univ., Lattakia, Syria

SOURCE: Organic Preparations and Procedures International (1979), 11(1), 17-22

CODEN: OPPIAK; ISSN: 0030-4948

DOCUMENT TYPE: Journal

LANGUAGE: English

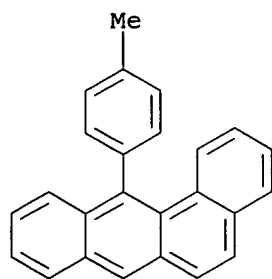
OTHER SOURCE(S): CASREACT 90:203754

IT 2498-65-9 70232-67-6 70232-69-8

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with aluminum chloride)

RN 2498-65-9 HCAPLUS

CN Benz[a]anthracene, 12-(4-methylphenyl)- (9CI) (CA INDEX NAME)

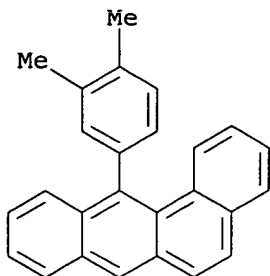


RN 70232-67-6 HCAPLUS

Young, Shawquia

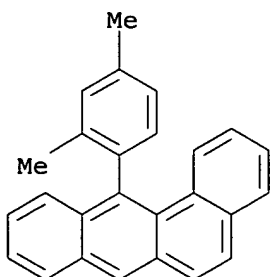
09/06/2006

CN Benz[a]anthracene, 12-(3,4-dimethylphenyl)- (9CI) (CA INDEX NAME)



RN 70232-69-8 HCAPLUS

CN Benz[a]anthracene, 12-(2,4-dimethylphenyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 11 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 22 Apr 2001

AB Studies on 107 polycyclic compds. of known carcinogenicity indicate that there is little relation between carcinogenicity and charge-transfer complex formation as measured by iodine, chloranil, trinitrobenzene, or acridine tests but there is a pos. relation between carcinogenicity and photodynamic action as measured with Paramecium.

ACCESSION NUMBER: 1965:17608 HCAPLUS

DOCUMENT NUMBER: 62:17608

ORIGINAL REFERENCE NO.: 62:3196d

TITLE: Charge-transfer complex formation, carcinogenicity, and photodynamic activity in polycyclic compounds

AUTHOR(S): Epstein, Samuel S.; Bulon, Inna; Koplan, Jeffrey; Small, Myra; Mantel, Nathan

CORPORATE SOURCE: Harvard Med. School, Boston, MA

SOURCE: Nature (London, United Kingdom) (1964), 204(4960), 750-4

CODEN: NATUAS; ISSN: 0028-0836

DOCUMENT TYPE: Journal

LANGUAGE: English

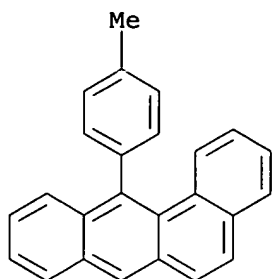
IT 2498-65-9, Benz[a]anthracene, 12-p-tolyl-
(carcinogenic action of, photodynamic action and)

RN 2498-65-9 HCAPLUS

CN Benz[a]anthracene, 12-(4-methylphenyl)- (9CI) (CA INDEX NAME)

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09/06/2006



L4 ANSWER 12 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 22 Apr 2001
GI For diagram(s), see printed CA Issue.
AB cf. C.A. 50, 8578e. Ice water (2 l.) added to 2.5 kg. 4% Na amalgam and then with stirring during 0.5 hr. 60 g. fluorenone-1-carboxylic acid (I) (orange needles, m. 191°) while maintaining the pH of the liquid near 7 by the slow addition of HCl, the mixture heated 4 hrs. on the steam bath, cooled, filtered, and acidified with 10% H₂SO₄, and the precipitate recrystd. from EtOH gave 30 g. fluorene-1-carboxylic acid (II), m. 245°; the mother liquor diluted with H₂O gave an addnl. 14 g. II. II (3 g.) treated at -10° with 5 g. CH₂N₂ in Et₂O, allowed to stand 12 hrs. at room temperature, and distilled yielded 3 g. Me ester of I, b_{0.8} 150°, m. 42°, d₂₇ 1.1250, n_{D27} 1.5652, MRD 66.12. An attempt to reduce I by the method of Huang-Minlon gave 100% (C.A. 47, 1649a) III, colorless needles, m. 262° (from BuOAc). II (30 g.) and 180 g. SOCl₂ refluxed 2 hrs. and evaporated in vacuo, the residue dissolved in C₆H₆ and evaporated to dryness in vacuo, and this procedure repeated several times gave 30 g. chloride (IV) of II, colorless needles, m. 108° (from C₆H₆). Pure H passed with stirring through 5 g. IV in 50 cc. boiling dry xylene containing 0.7 g. 10% Pd-C and 0.1 cc. Rosenmund inhibitor during 1.5 hrs., the mixture refluxed 0.5 hr., the xylene removed in vacuo, the residue distilled, and the distillate, b_{0.85} 158°, recrystd. from cyclohexane yielded 3.5 g. fluorene-1-aldehyde (V), colorless needles, m. 72°; 2,4-dinitrophenylhydrazone, orange-red needles, m. 262° (from EtNO₂). V (3 g.), 1.6 g. CH₂(CO₂H)₂, 1.2 g. pyridine, and 3 drops piperidine heated 4 hrs. on the steam bath and 5 min. at 150°, the mixture poured into 100 cc. H₂O and 5 cc. concentrated HCl, and the precipitate isolated gave 3.5 g. 3-(1-fluorenyl)acrylic acid (VI), long, colorless needles, m. 254° (from glacial AcOH). VI (3 g.) in 150 cc. dioxane hydrogenated at room temperature and 3 atmospheric pressure over 100 mg. PtO₂ yielded 100% 3-(1-fluorenyl)-propionic acid (VII), colorless needles, m. 205° (from glacial AcOH). VII (2 g.) and 60 g. polyphosphoric acid heated 2 hrs. with stirring at 120-30°, poured into 200 cc. cold H₂O, and extracted with Et₂O, and the extract worked up gave 1.2 g. 3'-oxo-1,2-cyclopentenofluorene (VIII), yellowish needles, m. 185° (from iso-PrOH). VIII (1.3 g.), 1.4 g. KOH, 2 cc. 85% N₂H₄.H₂O, and 10 cc. (CH₂OH)₂ treated by the method of Huang-Minlon (loc. cit.), diluted with 15 cc. H₂O, acidified with 4 cc. 6N HCl, and extracted with CHCl₃ gave 1.1 g. 1,2-cyclopentenofluorene (IX), white leaflets, m. 120° (from EtOH). MeMgI (from 0.6 g. Mg and 3.3 g. MeI) in Et₂O treated with 1.7 g. solid VIII, the Et₂O removed and replaced by C₆H₆, the mixture refluxed 4 hrs., kept 12 hrs. at room temperature, and decomposed with ice and H₂SO₄, and the C₆H₆ layer worked up gave 100% 3'-methyl-1,2-cyclopentadienofluorene (X), yellow crystals, m. 197° (from glacial

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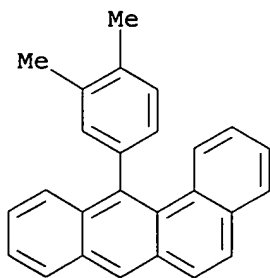
09/06/2006

AcOH). X (1 g.) in 100 cc. absolute EtOH hydrogenated at 2 atmospheric over 100 mg.

PtO2 gave 100% 3'-methyl-1,2-cyclopentenofluorene, colorless crystals, m. 121° (from glacial AcOH). 1,2,3,4-Tetrahydro derivative (2 g.) of II in 100 cc. absolute EtOH hydrogenated at slightly elevated temperature over 100 mg.

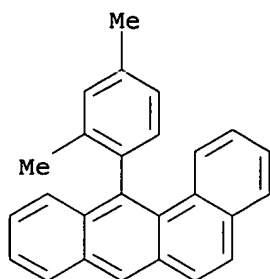
PtO2 yielded 1,2,3,4,1a,4a-hexahydro derivative of II, m. 138-9° (from cyclohexane). 2-Benzylcyclohexanone, b4 164-6°, m. 53-4°, cyclodehydrated with AlCl3 gave 40% 1,2,3,4-tetrahydrofluorene (XI), b6 135-40°, d27.5 1.0189, nD27.5 1.5600, MRD 54.02, silvery leaflets, m. 57° (from MeOH), and a considerable amount of resinous material; a liquid by-product, XI or an isomer, b0.4 82-4°, d25 1.0035, nD25 1.5533, MRD 54.10, was also obtained. XI (8 g.), 7 g. p-ClC6H4CHO, 1 g. piperidine, and 1 g. powdered KOH heated azeotropically in 50 cc. xylene, the solution washed with dilute acid, aqueous NaHCO3, and H2O, dried, and distilled gave some unchanged XI and then the 9-(p-chlorobenzylidene)derivative of XI, b0.09 210-15°, beautiful lemon-yellow prisms, m. 114-15°. XI (1.65 g.) in 100 cc. absolute EtOH hydrogenated over 100 mg. PtO2 gave 1,2,3,4,1a,-4a-hexahydrofluorene, colorless oil, b0.8 98°, nD26 1.5409.

ACCESSION NUMBER: 1956:77791 HCAPLUS
DOCUMENT NUMBER: 50:77791
ORIGINAL REFERENCE NO.: 50:14690b-i,14691a-b
TITLE: 1,2-Cyclopentenofluorenes and some derivatives of 1,2,3-4-tetrahydrofluorene
AUTHOR(S): Bergmann, Ernst D.; Ikan, Raphael
CORPORATE SOURCE: Hebrew Univ., Jerusalem
SOURCE: Journal of the American Chemical Society (1956), 78, 2821-4
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
IT 70232-67-6, Benz[a]anthracene, 12-[3,4-xylyl]- 70232-69-8
, Benz[a]anthracene, 12-[2,4-xylyl]-
(preparation of)
RN 70232-67-6 HCAPLUS
CN Benz[a]anthracene, 12-(3,4-dimethylphenyl)- (9CI) (CA INDEX NAME)



RN 70232-69-8 HCAPLUS
CN Benz[a]anthracene, 12-(2,4-dimethylphenyl)- (9CI) (CA INDEX NAME)

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L4 ANSWER 13 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 22 Apr 2001

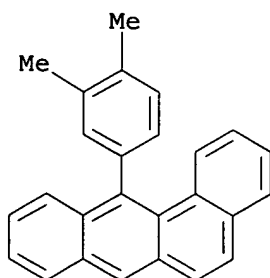
AB The Grignard reagent from 3.7 g. Mg and 30 g. 2,4,6-Me₃C₆H₂Br in 200 cc. dry Et₂O (initiated with EtMgI) refluxed 8 hrs., the Et₂O replaced with 12 g. o-(2-C₁₀H₇CH₂)C₈H₄CN in 200 cc. dry PhMe, the mixture refluxed overnight, treated with 30 cc. 20% aqueous NH₄Cl, and refluxed until cleared, the deep red, fluorescent liquid decanted, the residue washed with C₆H₆, and the combined PhMe and C₆H₆ solns. mixed with 20 cc. concentrated HCl gave 18 cc. crude 2-(1-naphthylmethyl)-2',4',6'-trimethyldiphenyl ketimine (I) HCl salt; the crude I treated with NaOH and extracted with C₆H₆ and the extract treated with concentrated HCl gave pure I.HCl, colorless crystals, m. 195° (decomposition) (from 1:10 EtOH-Me₂CO and 1:5 CHCl₃Et₂O). I.HCl (2.0 g.) in 25 cc. H₂O and 10 cc. concentrated H₂SO₄ heated 6 hrs. at 180° in a sealed tube, the resulting brown, glassy solid dissolved in 4:1 C₆H₆-petr. ether, the solution passed through Al₂O₃, and the percolate evaporated yielded 1.4 g. 2-(1-naphthylmethyl)-2',4',6'-trimethylbenzophenone (II), colorless crystals, m. 159.5° (from ligroine, 1:1 dioxane-EtOH, and Me₂CO). I.HCl (4.0 g.), 30 cc. AcOH, and 15 cc. 48% HBr heated 6 hrs. at 220° in a sealed tube, the product extracted with C₆H₆, and the extract chromatographed on Al₂O₃ gave 0.85 g. 1,2-benzanthracene (III), m. 157-8° (eluted with petr. ether); picrate, m. 140.5-1.5°; trinitrofluorenone adduct, m. 223-3.5°; further elution with 1:4 Et₂O-petr. ether gave 1.4 g. unidentified red oil. II (2.0 g.) and 15 g. Al₂O₃ heated 2 hrs. at 240-50° and 0.5 mm. and the mixture chromatographed yielded 1.5 g. 10-(2,4,6-trimethylphenyl)-1,2-benzanthracene (IV), colorless crystals, m. 144.5-5.5°. The 2,6-Me₂C₆H₃ analog (V) (2.0 g.) of I.HCl, 30 cc. AcOH, and 15 cc. 48% HBr heated 46 hrs. at 180° and worked up in the usual manner gave 0.40 g. III. V (1.5 g.) and 30 g. Al₂O₃ heated 3 hrs. at 240-70° and 1.0 mm. and chromatographed yielded 0.66 g. 2,6-Me₂C₆H₃ analog of IV, colorless crystals, m. 134.5-5.5°. The 2,6-Me₂C₆H₃ analog (VI) of II (2.0 g.), 30 cc. AcOH, and 15 cc. 48% HBr heated 21 hrs. at 180° yielded 0.63 g. III. VI (1.0 g.) and 25 g. Al₂O₃ heated 2 hrs. at 240-70° and 1.0 mm., the yellow powder chromatographed from 1:4 C₆H₆-petr. ether on Al₂O₃, a yellow fluorescent fraction rechromatographed from petr. ether on Al₂O₃, a colorless, blue fluorescent zone eluted, and the product recrystd. from EtOH yielded the dihydro derivative of 9-(2,6-dimethylphenyl)-1,2-benzanthracene (VII), colorless prisms, m. 193-200° (from EtOH); the mother liquor gave 6.0% VII, colorless plates, m. 123.5°, soluble in concentrated H₂SO₄ with red color which changed to blue and then brown. In the manner were prepared using Al₂O₃ the following analogs of IV (10-substituent and % yield given): Ph 99, o-MeC₆H₄ 82, m-MeC₆H₄ 92, p-MeC₆H₄ 96; and the following analogs of VII (9-substituent and % yield given): Ph 74, o-MeC₆H₄ 42, m-MeC₆H₄ 80, 2,4-Me₂C₆H₃ 75, 2,5-Me₂C₆H₃ 46, 3,4-Me₂C₆H₃ 68.

ACCESSION NUMBER: 1956:77790 HCAPLUS

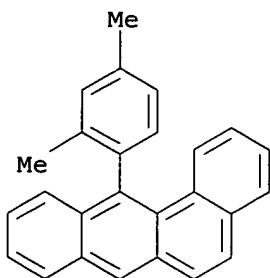
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09/06/2006

DOCUMENT NUMBER: 50:77790
ORIGINAL REFERENCE NO.: 50:14689e-i,14690a-b
TITLE: Use of alumina in aromatic cyclodehydration
AUTHOR(S): Vingiello, Frank A.; Borkovec, Alexej
CORPORATE SOURCE: Virginia Polytech. Inst., Blacksburg
SOURCE: Journal of the American Chemical Society (1956), 78, 3205-7
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
IT 70232-67-6, Benz[a]anthracene, 12-[3,4-xylyl]- 70232-69-8
, Benz[a]anthracene, 12-[2,4-xylyl]-
(preparation of)
RN 70232-67-6 HCAPLUS
CN Benz[a]anthracene, 12-(3,4-dimethylphenyl)- (9CI) (CA INDEX NAME)



RN 70232-69-8 HCAPLUS
CN Benz[a]anthracene, 12-(2,4-dimethylphenyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 14 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 22 Apr 2001
AB The Grignard derivative prepared from 63 g. 2,6-Me₂C₆H₃I and 6.6 g. Mg in 300 cc. dry Et₂O, the Et₂O replaced with 36.5 g. o-(2-C₁₀H₇CH₂)C₆H₄CN in 300 cc. dry PhMe, the mixture refluxed overnight, decomposed with 30 cc. 20% aqueous NH₄Cl, and filtered, the yellow filter residue boiled 2 hrs. with 20% HCl, the resulting yellow ketimine salt decomposed with boiling 20% aqueous NaOH and extracted with C₆H₆, and the extract treated with concentrated HCl yielded 49 g.
2-(2-naphthylmethyl)-2',6'-dimethyldiphenylketimine HCl salt (I), small lemon-yellow prisms, m. 192° (decomposition) (all m.ps. are corrected). I (10 g.) in 50 cc. 40% H₂SO₄ heated 8 hrs. in a sealed tube at 180°, cooled to about 5°, and the brown solid washed with H₂O and

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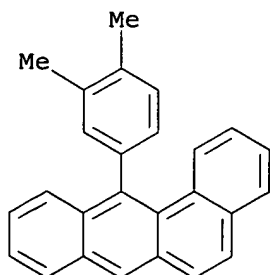
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recrystd. several times from EtOH gave 6.6 g. 2-(2-naphthylmethyl)-2',6'-dimethylbenzophenone (II), colorless prisms, m. 86.5-87° (from EtOH). The Grignard reagent prepared from 5.6 g. Mg, 43 g. 2,5-Me₂C₆H₃Br, and 250 cc. dry Et₂O, the Et₂O replaced by a solution of 37 g. I in 250 cc. dry PhMe, the mixture refluxed 5 hrs. and decomposed with 20% aqueous NH₄Cl, the

PhMe layer treated with concentrated HCl, the crystalline product mixed with 200 cc.

30% H₂SO₄ and 100 cc. PhMe and refluxed 7 hrs., and the PhMe layer worked up yielded 44 g. 2',5'-isomer of II, yellow viscous oil, b_{1.0} 236-8°. Similarly were prepared the following isomers of II (positions of Me groups, % yield, and b_{1.0} given): 2',3', 77, 240-3°; 2',4', 53, 235°; 3',4', 80, 238°; 3',5' (III), 82, - [m. 124.5-25° (from EtOH)]. III (2.0 g.), 20 cc. AcOH, and 10 cc. 48% HBr heated 4 hrs. at 180° in a sealed tube, cooled, extracted with C₆H₆, and chromatographed on Al₂O₃ with petr. ether yielded 1.5 g. 9-(3,5-dimethylphenyl)-1,2-benzanthracene (IV), m. 230°; further elution with C₆H₆-petr. ether and then with C₆H₆ gave 0.10 g. unidentified yellow material and 0.25 g. unidentified, deeply red material. In the same manner were prepared the following isomers of IV (position of Me groups, % yield, and m.p. given): 2,3, 34, 152-3°; 2,4, 75, 58-64° (colorless glassy solid); 2,5, 34, 64-9° (colorless glassy solid); 2,6, 6, 123.5°; 3,4, 65, 120-20.5° (from EtOH) (a 2nd polymorphic form, m. 142-3°, was also obtained from EtOH; both forms gave in concentrated H₂SO₄ red solns. which turned greenish brown after long standing).

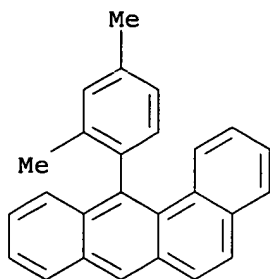
ACCESSION NUMBER: 1956:73858 HCAPLUS
DOCUMENT NUMBER: 50:73858
ORIGINAL REFERENCE NO.: 50:13855c-g
TITLE: Synthesis of the six isomeric 9-dimethylphenyl-1,2-benz-anthracenes
AUTHOR(S): Vingiello, Frank A.; Borkovec, Alexej
CORPORATE SOURCE: Virginia Polytech. Inst., Blacksburg
SOURCE: Journal of the American Chemical Society (1956), 78, 1240-2
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
IT 70232-67-6, Benz[a]anthracene, 12-[3,4-xylyl]- 70232-69-8
, Benz[a]anthracene, 12-[2,4-xylyl]-
(preparation of)
RN 70232-67-6 HCAPLUS
CN Benz[a]anthracene, 12-(3,4-dimethylphenyl)- (9CI) (CA INDEX NAME)



RN 70232-69-8 HCAPLUS
CN Benz[a]anthracene, 12-(2,4-dimethylphenyl)- (9CI) (CA INDEX NAME)

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09/06/2006



L4 ANSWER 15 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 22 Apr 2001

AB The synthesis of 4 new ketimine HCl salts, 4 new ketones, and 3 new hydrocarbons has been accomplished by the method described previously (C.A. 50, 3375c). Bradsher's aromatic cyclodehydration reaction (cf. C.A. 34, 2835.9) has been extended to the 9-aryl-1,2-benzanthracene system. The Grignard derivative from 11.6 g. Mg, 100 g. 2-ClC6H4Br, and 250 cc. Et2O treated with 65 g. 6-ClC6H4CHO, the mixture treated with 50 cc. 20% aqueous NH4Cl and extracted with Et2O, the extract washed, dried, and evaporated, and

the

residue fractionated gave 71 g. 2-chlorophenyl-2-naphthylcarbinol, b1.5 208-10°, b1 200-1°. C10H8 (384 g.), 650 cc. PhNO2, and 6 g.

AlCl3 treated at 30 mm. pressure with stirring with 242 g. o-ClC6H4CH2Cl, the mixture decomposed with 100 cc. 20% HCl, washed with H2O, dried, and evaporated, and the residue fractionated yielded 230 g. mixture (I) of 2- and 1-(o-ClC6H4CH2)C10H7, b10 220-3°. I (200 g.), 100 g. CuCN, 60 cc.

pyridine, and 0.2 g. CuSO4 heated 17 hrs. at 260°, the mixture cooled and distilled at 1 mm., the distillate poured into about 500 cc. 1:1 NH4OH, stirred, and extracted with Et2O, the extract washed with 2N HCl and H2O,

dried,

and distilled, the distillate (178 g.), b1 190-2°, dissolved in hot 90% EtOH, cooled to room temperature, seeded, and refrigerated 2 days, and the deposit filtered off gave 36 g. 2-(o-NCC6H4CH2)C10H7 (II), m.

80-4°; the filtrate concentrated and the residue recrystd. gave an addnl.

29 g. II; the crude II recrystd. twice from EtOH yielded pure II, m.

84-5°. The Grignard reagent from 12.9 g. o-BrC6H4Me and 1.8 g. Mg in 150 cc. dry Et2O concentrated and treated with 12.2 g. II in 100 cc. dry PhMe, the mixture refluxed 6 hrs. with stirring, cooled, and treated with an equivalent amount 20% NH4Cl, the PhMe decanted, the residue extracted with

C6H6, the

combined decantate and C6H6 extract treated with concentrated HCl, and the

slightly

yellow solid precipitate (17.2 g.) washed with ligroine (b. 60-90°), Me2CO, and finally with 95% EtOH-Me2CO gave 2-(2-naphthylmethyl)-2'-methyldiphenylketimine HCl salt (III), slightly brown large prisms, m.

185° (decomposition). Similarly were prepared (% yield and m.p. given): 3'-Me isomer (IV) of III, 70, 175°; 4'-Me isomer of III, 55,

194°; 2-(2-naphthylmethyl)diphenylketimine HCl salt, 80, 181° (all compds. melted with decomposition). IV (10 g.), 40 cc. 25% H2SO4, and 30 cc. PhMe refluxed 2 hrs., the PhMe layer washed, dried, filtered through C, and evaporated, and the residue fractionated yielded 2-(2-naphthylmethyl)-3'-methylbenzophenone (V), viscous oil, b1.5

136-8°. Similarly were prepared (% yield and b.p./mm. given): 2'-Me isomer of V, 80, - (m. 88.5-9.5°); 4'-Me isomer of V, 86,

237-40°/1.5; 2-(2-naphthylmethyl)benzophenone, 99,

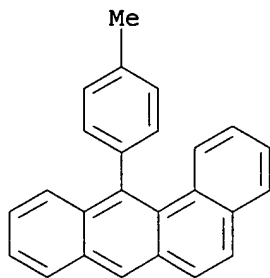
236-8°/1.3. V (1 g.), 15 cc. 48% HBr, and 30 cc. glacial AcOH

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09/06/2006

heated 3 hrs. in a sealed tube at 180°, the mixture extracted with C₆H₆, washed, dried, filtered, diluted with petr. ether, chromatographed on Al₂O₃, and eluted with petr. ether and then 30% C₆H₆-petr. ether, the combined percolates evaporated, and the residue recrystd. from EtOH-Me₂CO gave 0.90 g. 9-(3-methylphenyl)-1,2-benzanthracene (VI), colorless silky needles, m. 132.5-3.5°. Similarly were prepared (% yield and m.p. given): 2-Me isomer of VI, 80, 103.5-4.5°; 4-Me isomer of VI, 85, 116.5-17.5°; 9-phenyl-1,2-benzanthracene, 95, 154-5°.

ACCESSION NUMBER: 1956:31999 HCAPLUS
DOCUMENT NUMBER: 50:31999
ORIGINAL REFERENCE NO.: 50:6383b-i
TITLE: The synthesis of 9-phenyl-1,2-benzanthracene and the three isomeric 9-monomethylphenyl-1,2-benzanthracenes
AUTHOR(S): Vingiello, Frank A.; Borkovec, Alexej
CORPORATE SOURCE: Virginia Polytech. Inst., Blacksburg
SOURCE: Journal of the American Chemical Society (1955), 77, 4823-4
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 50:31999
IT 2498-65-9, Benz[a]anthracene, 12-p-tolyl- (preparation of)
RN 2498-65-9 HCAPLUS
CN Benz[a]anthracene, 12-(4-methylphenyl)- (9CI) (CA INDEX NAME)



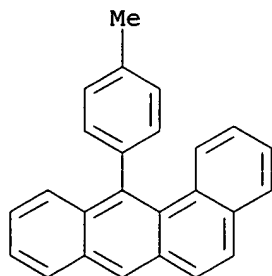
L4 ANSWER 16 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN
ED Entered STN: 22 Apr 2001
AB cf. C.A. 48, 3308h. Ellagic acid (I), a H₂O-soluble tannin-containing fraction, and a red pigment (II) were isolated from fresh timber shavings of E. diversicolor (III). II can be represented by the rounded average formula C₁₁₀H₁₁₀O₅₀, containing 18 phenolic and 7 other OH groups, 4 MeO, 1 CO, and 2 ester groups, while the other unreactive O atoms are likely to be in furan or pyran rings. Extraction of III with MeOH under N yields 1.6-2.3% crude II (IV) from which I tetraacetate could be isolated by crystallization from Me₂CO. If IV was washed with Et₂O to remove waxy materials and II acetylated with Ac₂O in pyridine, I tetra-acetate crystallized, while the brown II acetate separated on dilution with H₂O and yielded 4 fractions on chromatography on Al₂O₃ by elution with different solvent mixts. II with CH₂N₂ in MeOH at 0° gave the methylated pigment (V), m. above 240°, in which possibly 7 OH groups could be methylated with Ac₂O and pyridine to a product m. above 230°. V gave a monoxime, m. above 250°, with NH₂OH.HCl in pyridine. Hydrolysis of IV with H₂SO₄ showed no addnl. I in II, but hydrolysis of V with KOH in aqueous MeOH and Me₂CO indicated the

Young, Shawquia

09/06/2006

presence of 2 moles 3,4,5-(MeO)3C6H2CO2H in V by yielding a compound, m. above 190°, in which 2 further OH groups could be acetylated by Ac2O and pyridine at room temperature to a product m. above 180°. When V was stirred in hot Me2CO with Me2SO4 and NaOH, the product, m. above 290°, showed methylation of 2 further OH groups, formed possibly by hydrolysis of the 2 ester groups. Alkali fusion of II at 220-40° gave 3,4-(HO)2C6H3CO2H, while 3N HNO3 yielded NH4 tetroxalate. Demethylation of II with HI yielded phenolic products, but gave no crystalline benzoates. A pink specimen of E. regnans (VI) yielded 1.6% crude pigment, in which the red pigment differs slightly from that of II and which contains more I than III does; the normal VI contains even more I.

ACCESSION NUMBER: 1956:31998 HCAPLUS
DOCUMENT NUMBER: 50:31998
ORIGINAL REFERENCE NO.: 50:6382g-i,6383a-b
TITLE: Chemistry of Western Australian plants. IX.
Extractives from the timber of Eucalyptus diversicolor
AUTHOR(S): Michael, M.; White, D. E.
CORPORATE SOURCE: Univ. W. Australia, Nedlands
SOURCE: Australian Journal of Applied Science (1955), 6,
359-64
CODEN: AJACA3; ISSN: 0572-1156
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
IT 2498-65-9, Benz[a]anthracene, 12-p-tolyl-
(preparation of)
RN 2498-65-9 HCAPLUS
CN Benz[a]anthracene, 12-(4-methylphenyl)- (9CI) (CA INDEX NAME)



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ENTER NAME OR (END):end

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Executing the logoff script...

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COST IN U.S. DOLLARS	SINCE FILE	TOTAL
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	ENTRY	SESSION
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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-12.00	-12.00

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